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Title: Understanding Discrete Fracture Networks Through Spectral Graph Theory

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Understanding Discrete Fracture Networks Through Spectral Graph Theory

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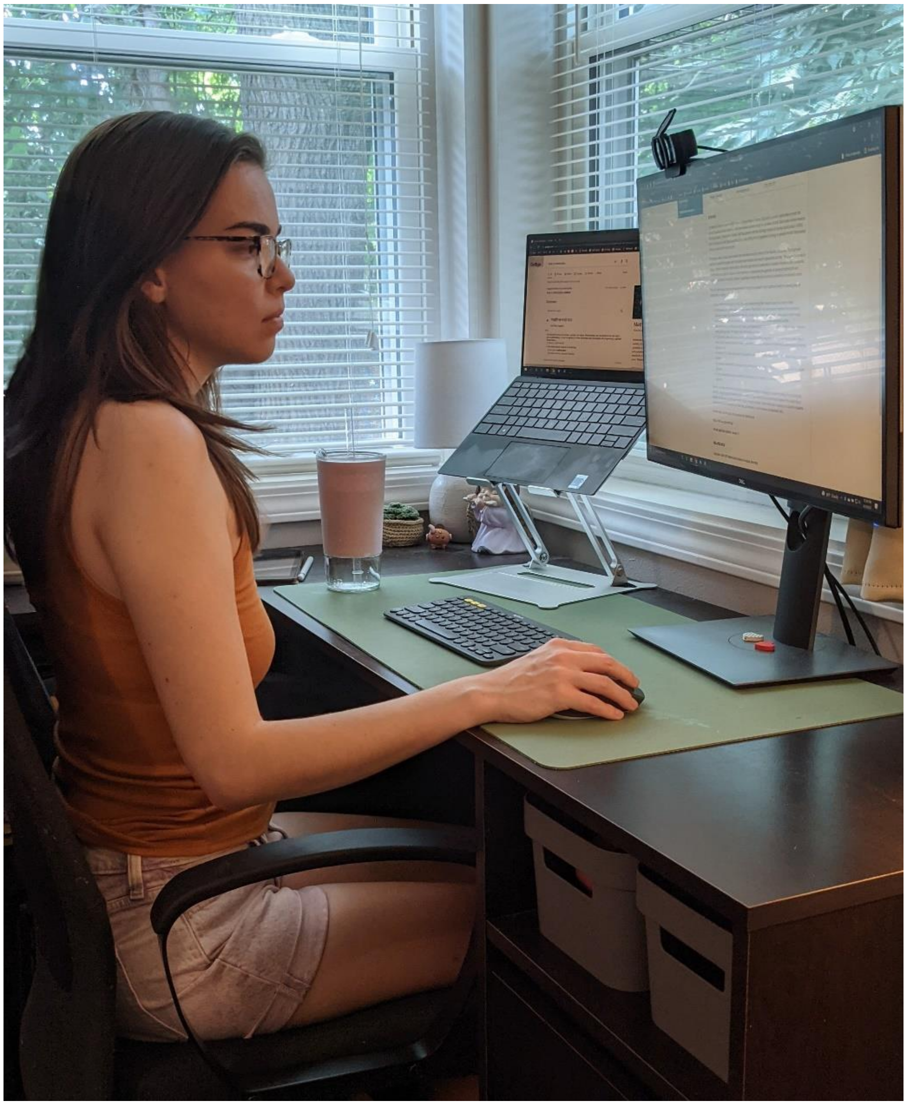
Abstract: Discrete Fracture Network models (DFNs) are used to simulate fluid flow and particle transport through fracture networks in low permeability rock. Understanding these processes are essential in many subsurface applications, such as environmental restoration of contaminated fractured media, CO_2 sequestration, detection of low-level nuclear tests, and hydrocarbon extraction. Compared with other models, DFNs allow for incorporation of a wider range of network characteristics but have substantially greater computation cost. These networks can be represented with graphs, allowing the use of graph theory tools to study the networks. I used Python to simulate flow and transport on a range of DFNs and analyzed these networks using methods from network analysis and spectral graph theory. My purpose was to find ways to gain insight about flow and transport on DFNs using these graph representations, bypassing the computationally intensive meshing typically required. My work is still in progress, but I have discovered several interesting trends and patterns that I believe could be useful towards my goal. If I am able to bring these results to fruition, they will aid subsurface geologists in extracting flow and transport information about fracture networks more efficiently.



Working at home during my virtual internship. Photo credit: Destry Newton.

Understanding Discrete Fracture Networks Through Spectral Graph Theory

Introduction

Discrete Fracture Networks (DFNs) are used to model fracture networks in low permeability rock. They allow simulation of fluid flow and particle transport on these networks. Understanding properties of flow and transport in fracture network is important in many areas, including climate management, nuclear testing detection, and environmental cleanup. The computation cost of DFN simulations is high, thus many efforts have been taken to reduce the computational demands while maintaining reliable results. DFNs can be represented by graphs, a process which extracts topological data about the networks, while forgetting geometric features. Graph representations have been used in a variety of ways to decrease the computational requirements for flow and transport simulations on DFNs. This summer, I was tasked with studying these graph representations from the perspective of spectral graph theory, looking for new ways to gain information about DFNs efficiently. This project appealed to me because of my interest in graph theory and topology. I enjoyed the opportunity to work with familiar concepts in a significantly more applied setting than I have previously experienced.

Description of the Research Project

Three-dimensional DFNs use two-dimensional shapes to model fractures in a three-dimensional domain. For my project, we chose to model the fractures using discs with radii sampled from the truncated power law distribution shown in equation 1. This aligns with what has been observed in field studies for some classes of rock.

$$\frac{\alpha}{1}\,\frac{\left(\frac{r}{1}\right)^{-1-\alpha}}{1-\left(\frac{25}{1}\right)^{-\alpha}},\ 1 \le r \le 25 \qquad (1)$$

I used the computational suite dfnWorks, designed by scientists at Los Alamos, to generate 30 such DFNs for each of ten values of α. Below are images of a few of the DFNs I generated for different values of α.

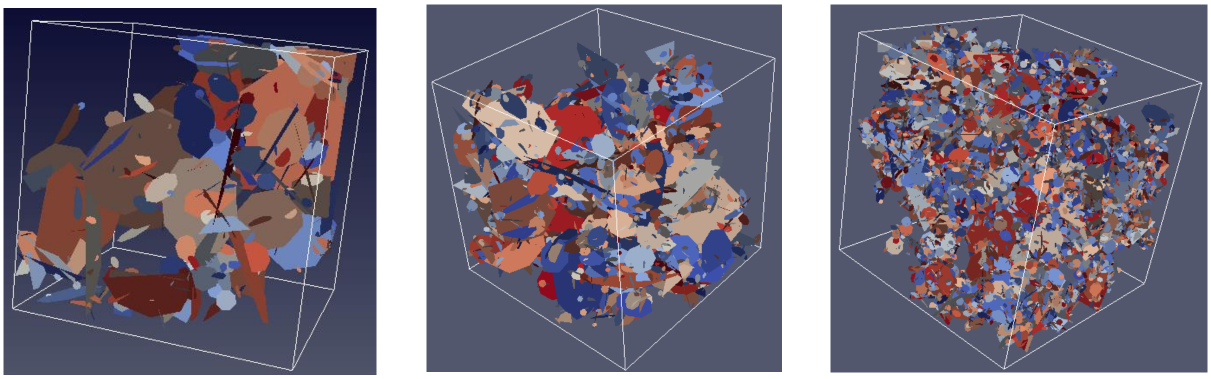


Figure 1: DFNs with α = 1.25, 2, and 2.75 (left to right)

In the images above, each disc (modeled by polygons) represents a fracture in the cubic rock mass outlined in white. I also generated graphs corresponding to each of my sample DFNs. There are three different graphs which have been used to model DFNs. The first, called the fracture graph has a vertex representing each fracture and an edge connecting each pair of vertices representing intersecting fractures. The intersection graph has a vertex representing each intersection between two fractures and an edge connecting two vertices if the intersections represented by the two vertices share a common fracture. Finally, there is a bipartite graph representation which contains a vertex representing each fracture and each intersection. There is an edge between two vertices in this graph if one vertex represents a fracture and the other vertex represents an intersection on that fracture. Figure 2 shows the fracture graph representing the DFN with α = 1.25 pictured above.

My task was to search for ways to use spectral graph theory to understand these graphs, with the goal of finding ways to gain information about these networks and properties of their flow and transport at a reduced computation cost. Spectral graph theory studies the eigenvalues of the

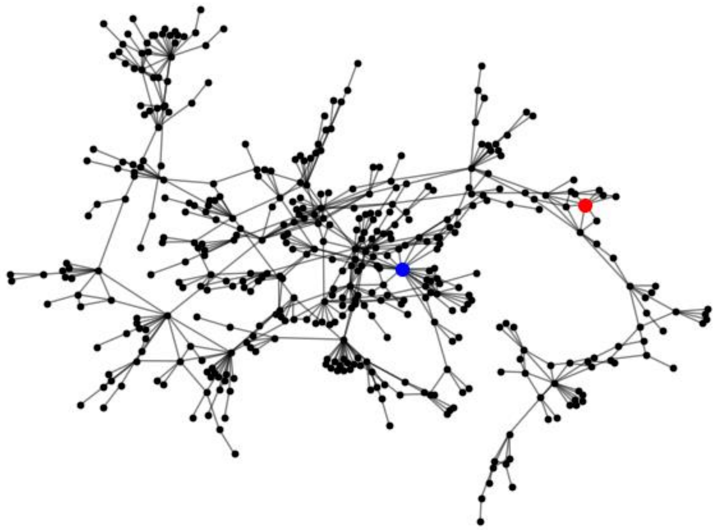


Figure 2: Fracture graph representing a DFN with α = 1.25

Laplacian operator associated with a graph. The Laplacian operator is a discrete version of the Laplacian operator on manifolds. It takes a real-valued function defined on the vertices of a graph and returns the gradient of the flux of this function. The range of the eigenvalues, the multiplicity of certain key eigenvalues, the least non-zero eigenvalue, and the general distribution of eigenvalues have been shown to reveal both local and global information about a graph. The eigenvalues of the adjacency matrix of a graph are also sometimes studied in spectral graph theory.

I used dfnWorks to simulate fluid flow and particle transport on the DFNs I generated. I compared the passage times of particles in networks generated with different values of α. See Figure 3. In this figure, there are noticeable differences between the initial and peak breakthrough times for different values of α.

I also calculated and plotted the Laplacian and adjacency spectra for each of the graphs associated to the DFNs I generated. The Laplacian spectra for my fracture graphs are shown in Figure 4. There is a noticeable decrease in the density of eigenvalue 1 as α increases. High multiplicity of eigenvalue 1 can indicate a high degree of local symmetries, which can be observed in our graphs.

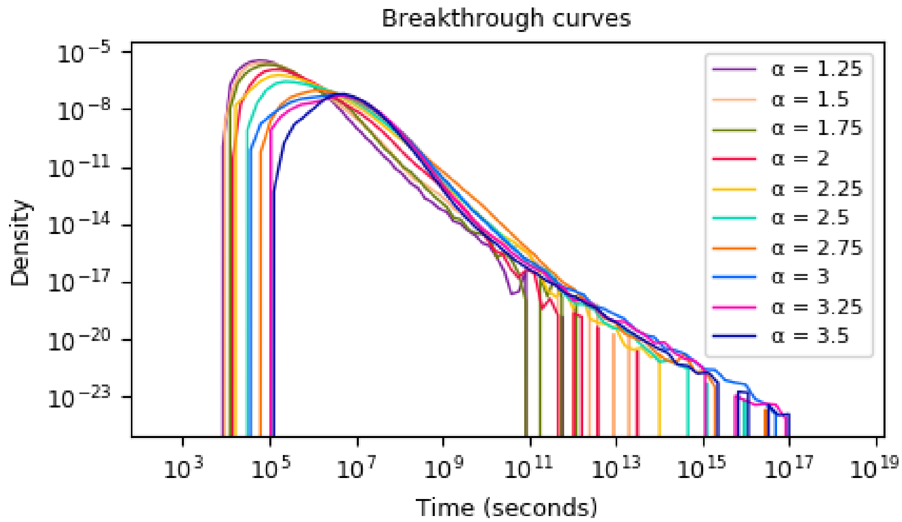


Figure 3: Breakthrough curves for DFNs generated using different values of α as the power law exponent

Finally, I calculated and plotted various other features of the graphs. See Figure 5 for an example. The source and target connectivity shown in this figure is a measure of the number of edges which must be removed in order to disconnect the inflow and outflow boundaries.

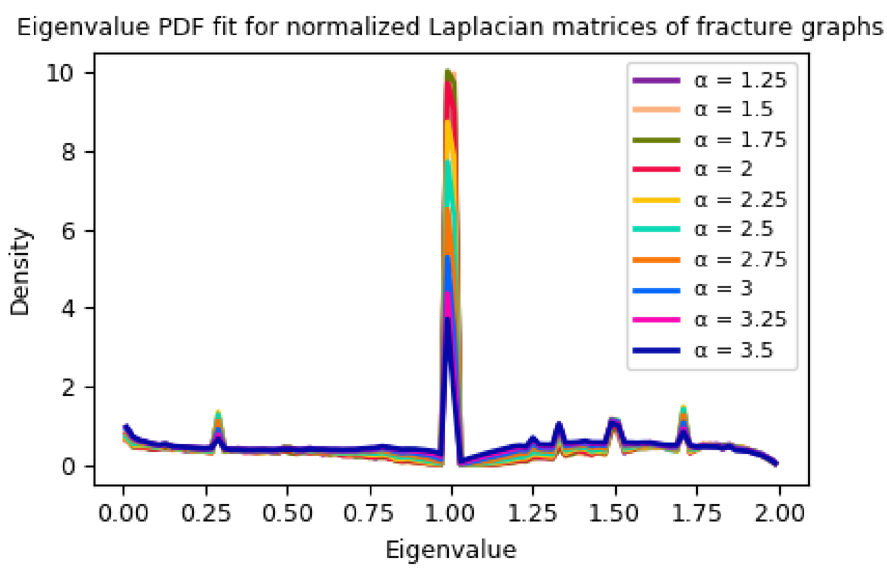


Figure 4: Laplacian spectra of fracture graphs of DFNs generated using different values of α as the power law exponent

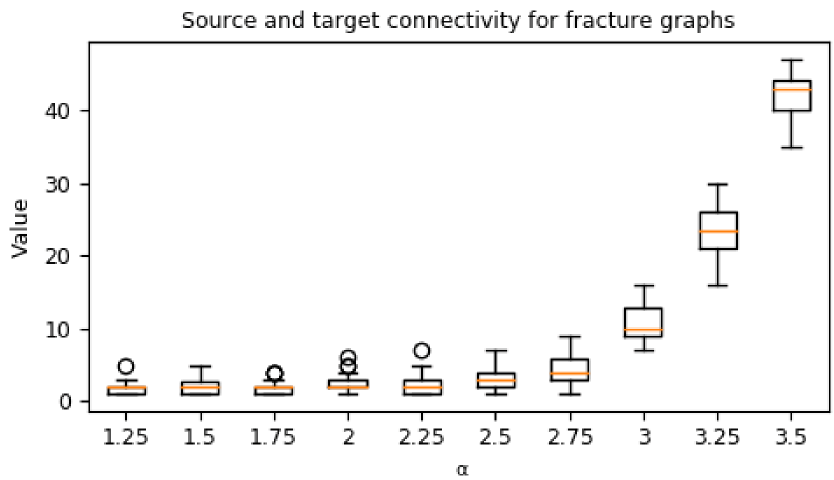


Figure 5: Source and target connectivity of DFNs generated using different values of α as the power law exponent

I am currently working to find connections between the breakthrough curves representing passage times of particles and graph properties. My hope is to be able to predict properties of flow and transport based on the graph spectrum.

Contributions Made to the Project

I wrote code in Python to generate the DFNs and associated graphs described above using the dfnWorks suite. I used the package NetworkX to calculate various information about these graphs, including information about their spectra, and I used the package Matplotlib to visualize my findings. I met regularly with my mentors to discuss my progress and decide on next steps. Additionally, I compiled a document with my findings. I included detailed information about the various statistics calculated, including their formal definitions, examples, intuition, and interpretation in the context of our graphs. I also spent time reading about spectral graph theory and included a substantial section in the document describing my findings. My hope is that this document is written in such a way so that the scientists at the lab can read and understand it, so that it might be of use to them if they choose to pursue further research in this direction in the future.

I gave a talk about my research at a seminar for my research group at the lab describing my progress on the project. I explained some background on the project, gave a brief introduction to spectral graph theory, and displayed some of the interesting plots I created. I discussed my hopes for the project should I be able to continue it in the future.

Skills and Knowledge Gained

Mathematically, I learned a significant amount about spectral graph theory and network analysis. I now understand central questions and results within these fields. I also gained practice translating between a physical system (fracture networks) and an abstracted system (graph representations).

I also made substantial gains in my programming abilities and confidence. I had previously coded for a few classes and occasionally on my own, but this was my first experience that required writing extensive code and developing the code over time. I've improved my ability to design complex functions and workflows. For the first time, I was forced to think about writing code efficiently. I gained experience with several commonly used python packages. Finally, I found that I can pick up new programming skills quickly and have a much higher confidence in my ability to learn new programming skills.

Additionally, I practiced using other tools essential to any computer scientist. I became much more comfortable using the command line. I learned basics of VIM and git. I also took advantage of LANL's computing resources, incorporating parallel processing and cluster computing to drastically reduce run times.

Because of the diverse backgrounds of those I worked with, I was required to take extra care to explain concepts in simple and clear ways. I often needed to find ways to share ideas with researchers of varying mathematical backgrounds. This requires effort and attention, and is an essential skill for anyone working in an interdisciplinary context.

Finally, I gained understanding about the daily working life of laboratory employees and a broader understanding of the overarching mission of Los Alamos National Laboratory. I discovered that there are many opportunities at LANL for researchers with quantitative backgrounds, and I have a much better understanding of how to develop and prepare myself for such a job.

Relevance to the Mission of NSF

Understanding fluid flow and particle transport in fracture networks in low permeability rock has a broad range of applications, as described above, including climate control, nuclear testing detection, and environmental safety. These applications are critical to advancing national security and global well-being. Currently, methods for simulating flow and transport in fracture networks can be very computationally intensive. It is my hope that the work I've done this summer can be used to find computationally cheaper ways to obtain the same information. This will aid scientists nationally and abroad in running more complex simulations and extracting more data about the applications at hand.

Research Experience Impact on Your Academic and Career Planning

I was quite surprised to discover how much I enjoyed my research project over the summer. Previously, my research has been very theoretical, with the only applications to other areas of theoretical math. I had become frustrated with my inability to see any of the fruits of my work. This summer, I was able to apply the mathematical skills I have developed as a graduate student to an applied problem, where not only could I clearly see why my research was important, but I could easily explain to others outside of academia why my work mattered. I found this very motivational and exciting.

I also particularly enjoyed the collaborative aspect of my internship. I have worked with others on research projects in the past, but typically with other researchers who have similar backgrounds to my own. The interdisciplinary nature of the collaboration on this project allowed everyone a unique perspective to contribute. I felt energized by the idea that I might have distinctive and important perspectives to contribute to the team.

During my internship, I was able to speak with many lab employees about their careers. Several employees lauded the work-life balance available to lab workers and the friendly professional environment. I learned that many of the stressors which plague the careers of other PhD holders are less prevalent in national lab jobs, allowing a more relaxed and focused work atmosphere. I believe that a national lab job is an excellent fit for my work style, priorities, and ambitions.

As a result of my enjoyment of the internship, I plan to further develop skills for applied research, such as programming, machine learning, and data analysis. I registered for a deep learning class for the fall semester and hope to do reading about topological data analysis. I desire to take advantage of the numerous opportunities at my university to enhance these critical skills over the coming years.

Further, I plan to shift my research direction to help me focus these abilities. Previously, my work featured a minimal computational component, but in the future, I desire to incorporate computation more centrally. I have already discussed these plans with my PhD advisor and have several ideas about work to do in this direction.

Finally, if I continue to enjoy working on more applied mathematics problems, I plan to apply for a postdoc position at a national lab once I approach my graduation date. I believe it would be an enjoyable, suitable, and rewarding next step for me.

Acknowledgements

I would like to thank my host institution, Los Alamos National Lab, for their willingness to let me engage in research with them. The lab provided many opportunities to meet other students and lab employees, learn about research and job opportunities, and develop as a professional.

I would also like to thank my mentors Jeffrey, Matt, and Aric for the considerable amount of guidance, encouragement and time they provided to me over the course of my internship. It was truly a pleasure to work with them.

Finally, I'd like to thank my PhD advisor Chris Leininger for being exceedingly supportive about my pursuit of the internship, and Chandrika Sadanand and Sarah Mousley Mackay for their assistance along the way.

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